

All Available Peripheral Moiety Precursors

31

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Chemists Select
Initial Set of k Peripheral Moiety Precursors

37

Computer selected set
of peripheral moiety
precursors

Apply Mass Coding
Algorithms

35

Generate all subsets of k peripheral
moiety precursors and calculate the
mass redundancies of the resultant
libraries. Pass only those subsets of k
peripheral moieties that yield mass
coded libraries

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Subsets of k peripheral moiety
precursors that yield mass
coded libraries

41

Figure 1A: Mass Coding Flowchart

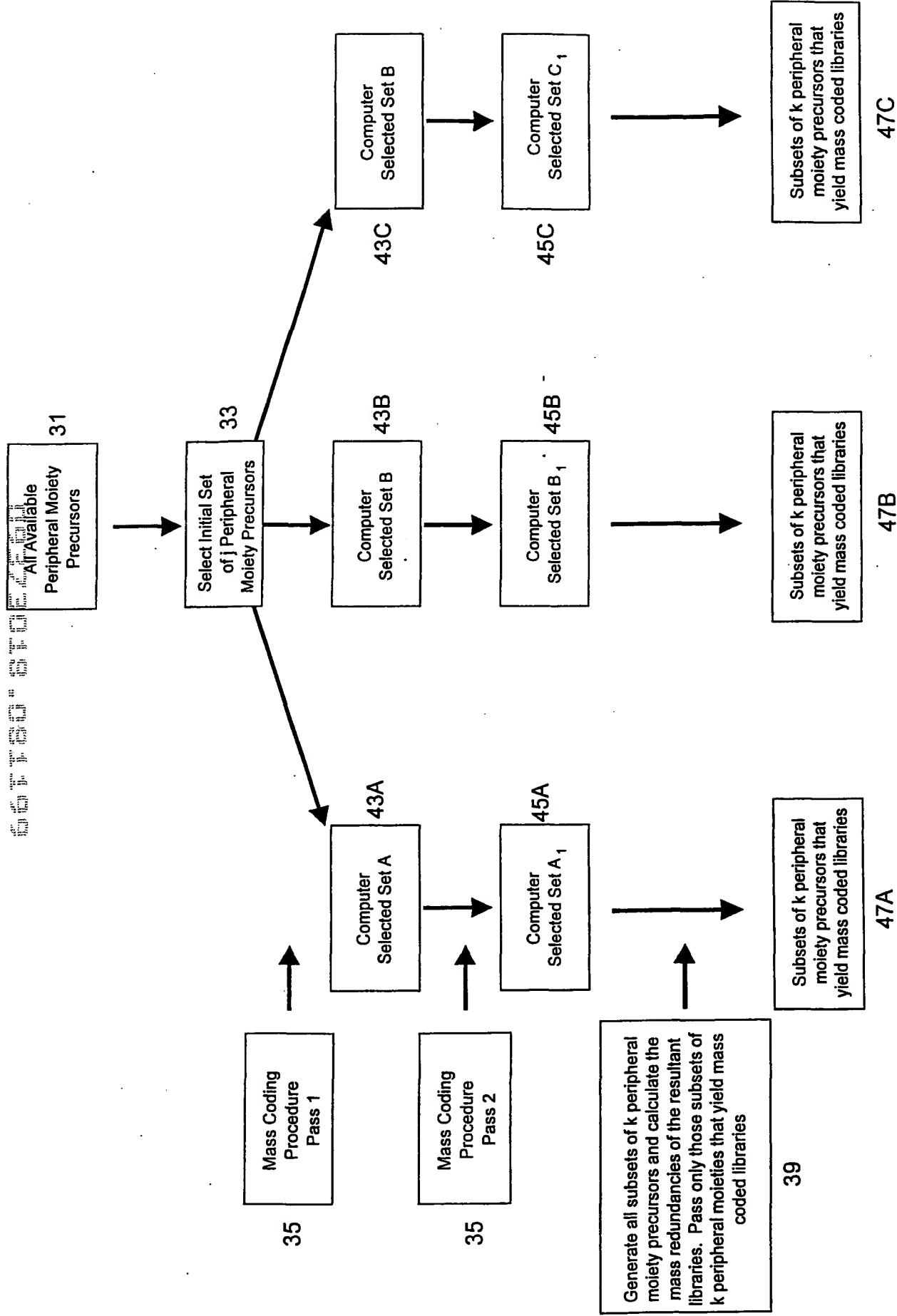


Figure 1B: Alternate Method for Mass Coding

Figure 2: Statistical Analysis of the Percentage Mass Redundancy of Libraries Obtained From Either a Computer Selected Set of Peripheral Moiety Precursors or From a Randomly Chosen Set of Peripheral Moiety Precursors

Fig: 2A

% Mass Redundancy of Libraries
From a Computer Selected Set of
Peripheral Moiety Precursors

Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	24	1.32
<5%	234	12.86
<10%	972	53.41

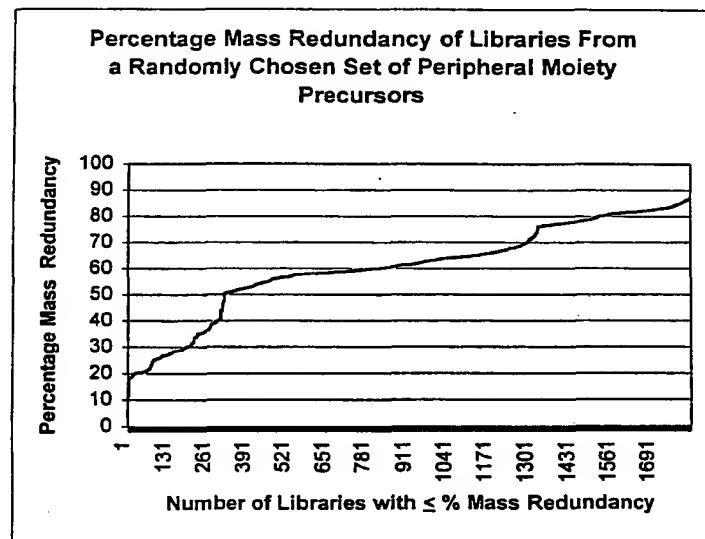
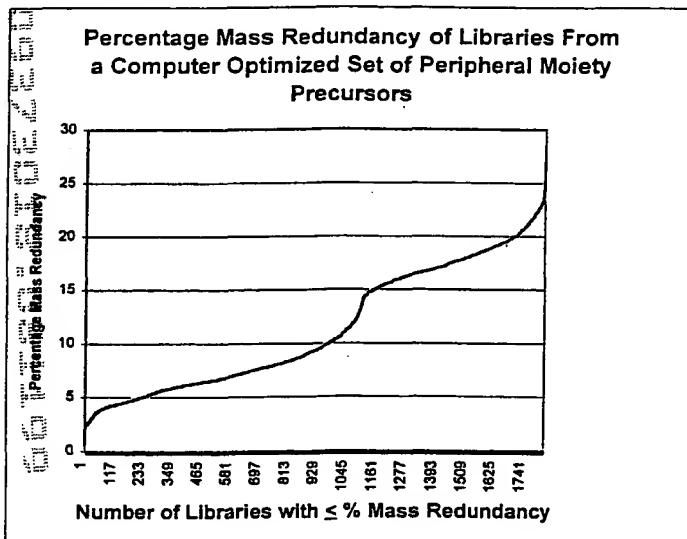
Average Mass Redundancy 11.47 Percent

Fig: 2B

% Mass Redundancy of Libraries
From a Randomly Chosen Set of
Peripheral Moiety Precursors

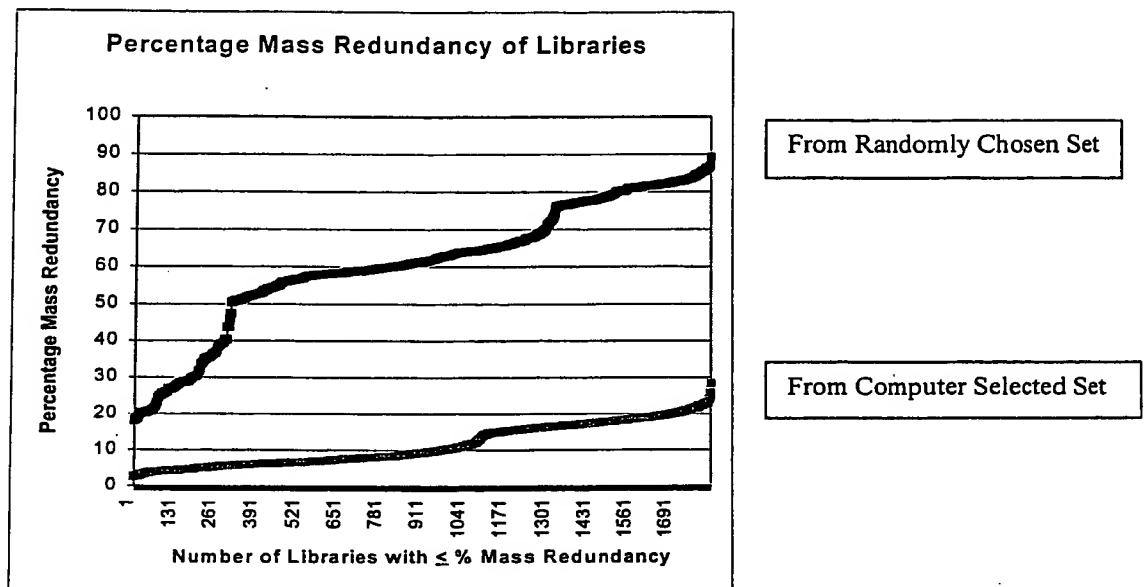
Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	0	0.00
<5%	0	0.00
<10%	0	0.00

Average Mass Redundancy 60.69 Percent



¹ Note: Y-ordinate scale is different for two charts.

Figure 2C: Comparison of the Percentage Mass Redundancy of Libraries Obtained From a Computer Selected Set of Peripheral Moiety Precursors vs. Those Obtained From a Randomly Chosen Set of Peripheral Moiety Precursors



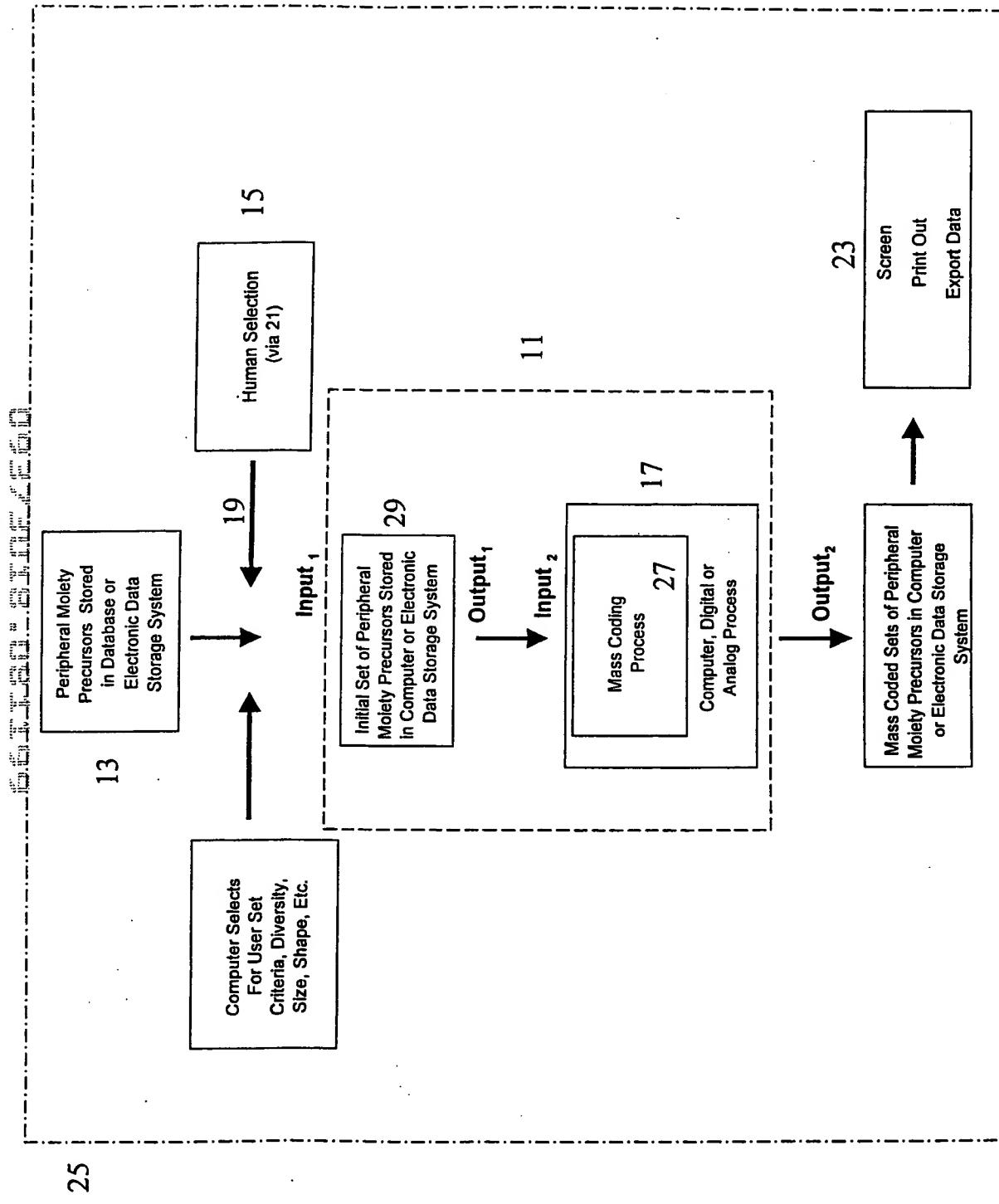


Figure 3: System Flow for Mass Coding Process